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A TRAPPED ELECTRON MODEL FOR APPLICATION TO THE MACH CODE

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A method has been developed for modeling the space charge density due to electrons trapped in a potential energy well, and produces stable solutions using the MACH code. The trapped electrons are assumed to thermalize due to collisions with the source electrons, and reach an equilibrium distribution which depends on the well depth. The model has one free parameter, and requires evaluation of a quadrature. The basic equations and some numerical results are presented. A comparison of a plasma chamber simulation is given, using the model and measured data.

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1. INTRODUCTION

In order to produce stable solutions using the MACH code [*Tautz, et. al.*, 1987] for the Multiple Interactions in Plasma (MIP) chamber experiment simulations [*Morgan, et. al.*, 1989; *Chan, et. al.*, 1989], it was found necessary to include a trapped electron model. The physical assumptions and the numerical techniques used to implement this model are presented in this report.

We first describe the nature of the instability that is encountered in the chamber simulations if the trapped electrons are absent. The source of this instability is illustrated schematically in Figure 1. The ion beam enters the chamber at the throat and creates a region of positive charge. This positive space charge attracts electrons from the neutralizing source near the throat entrance, causing the electron density to decrease (for strictly one-dimensional motion, the density falls off inversely as the square root of the potential). On the other hand, the ions are repelled by the positive charge and tend to build up at the turn-around point, thereby increasing the ion density. These two effects produce a region of increasing net positive charge which does not stabilize until a wall of positive potential builds up to the stagnation energy of the ions. At this point, the potential would shut off the beam ion current. Since this phenomena is not observed in the chamber, it must be an unphysical effect due to the neglect of some essential physics component.

The MACH program normally proceeds to find solutions by Poisson-Vlasov iteration, i.e. the plasma is assumed to be collisionless. (The code was designed for space simulations, where this can be a good approximation.) However, when applied to the MIP chamber simulations, the above instability problem was encountered. To achieve reasonable, stable solutions, we have included collisional effects for the electrons. That is, we assume some electrons will scatter into the potential energy well that is created by the streaming ions, and quench the unstable region of positive charge. We further assume that the electrons establish an isotropic equilibrium within the well, with temperature equal to that of the Vlasov (untrapped) electrons. The details of this trapped electron model are described below. In section 2, we outline the "usual" method of obtaining density in MACH by means of inside-out trajectories and velocity space quadratures. This serves to introduce the basic equations and notation. In section 3, we describe the modifications which enable us to calculate the density of the trapped electrons. An approximate expression for the untrapped population is also given. Density normalization of the untrapped component is determined by equating ion and electron fluxes in the source region. The normalization constant for the trapped component is essentially a free parameter of the model. In section 4, we give some numerical results for the model for MIP experiment simulation. The conclusions are presented in section 5.

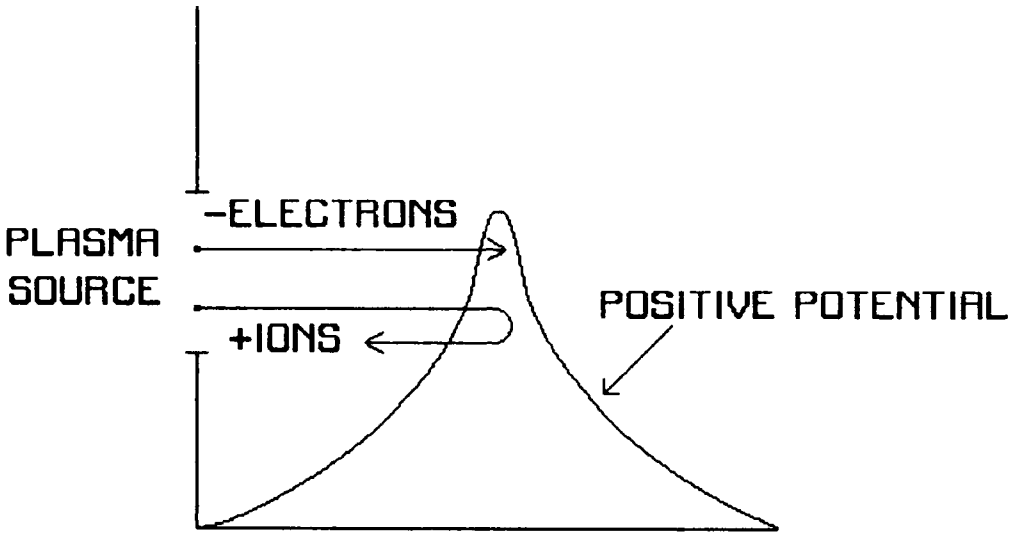

Figure 1. Schematic of instability in electrostatic potential

2. THE INSIDE-OUT METHOD

In the MACH program, the dimensionless particle number density $n = N/N_\infty$ is calculated by a velocity space integral over the distribution function $f(\vec{v})$ at every point $\vec{r}$ of the spatial grid

$$n = \iiint f(\vec{v})\, d\vec{v}$$

$$= \iiint f(v,\theta,\phi)\, v^2\, dv\, d\Omega$$

where $d\Omega$ is the solid angle element

$$d\Omega = \sin(\theta)\, d\theta\, d\phi$$

We now make a transformation from velocity v to total energy E, given by

$$E = \frac{1}{2} m v^2 + qV$$

where $V = V(\vec{r})$ is the local electrostatic potential. By differentiating this equation, we get

$$dE = m v\, dv$$

so that

$$v^2\, dv = v/m\, dv = 2^{1/2} m^{-3/2} (E - qV)^{1/2}$$

and the density integral goes into

$$n = 2^{1/2} m^{-3/2} \iiint f(E,\theta,\phi)(E - qV)^{1/2}\, dE\, d\Omega$$

By Liouville's theorem, the distribution function is constant along a particle trajectory, so that by following time-reversed tracks to infinity, we can obtain $f(E, \theta, \phi) = f_\infty$. If we now specialize to a drifting Maxwellian distribution at infinity, we can write f_∞ as

$$f_\infty = (m/(2\pi k T))^{3/2} \exp(-X)$$

where the exponent has the form

$$X = \frac{1}{2} m(\vec{v}_\infty - \vec{v}_s)^2/kT$$

$$= e + M^2 - 2e^{1/2} \cdot M \cdot \cos(\theta_\infty)$$

and

$\vec{v}_\infty$ = *track velocity at infinity*
θ_∞ = *track polar angle at infinity*
$\vec{v}_s$ = *source flow velocity at infinity*
$e = E/kT = \frac{1}{2} m(\vec{v}_\infty)^2/kT$
$M = v_s/(2kT/m)^{1/2}$ = *Mach number*

Using these variables, we can write n as

$$n = \frac{1}{2}\pi^{-3/2} \iiint \exp(-X)(e-\chi)^{1/2} de\, d\Omega$$

where $\chi = qV/kT$ is the dimensionless potential energy. This is the expression used in MACH to calculate density by means of quadratures. In order to evaluate the integrand of the triple integral, particles are tracked backwards in time to the source to obtain θ_∞ and hence f_∞ (any particles hitting objects contribute zero density). This tracking must be done for each value of e, θ, ϕ with sufficient precision to resolve the distribution function over all energies and 4π solid angle. (In practice, we have developed the VSTS method so that these orbits may be selected efficiently.) What is of interest to us here is the energy range for the particles.

Figures 2 and 3 depict the energy diagrams for repulsive and attractive potentials. The horizontal lines show typical energy bins for tracking, which are set to span, with sufficient accuracy, the Mach energy M^2 at infinity. The kinematic constraint that the kinetic energy $k = e - \chi$ be greater than zero sets the integration limits on total energy:

repulsive potential $(\chi > 0)$: $0 \le e \le \infty$
attractive potential $(\chi < 0)$: $\chi \le e \le \infty$

Although the total energy range χ to 0 is kinematically allowed for attractive potentials, it is normally excluded from the MACH calculations because such orbits cannot connect to infinity, i.e. they are energetically trapped. The only way that these orbits can become populated is by collisions. The trapped electron model fills in this kinematic region with an approximate equation, which is described in the next section.

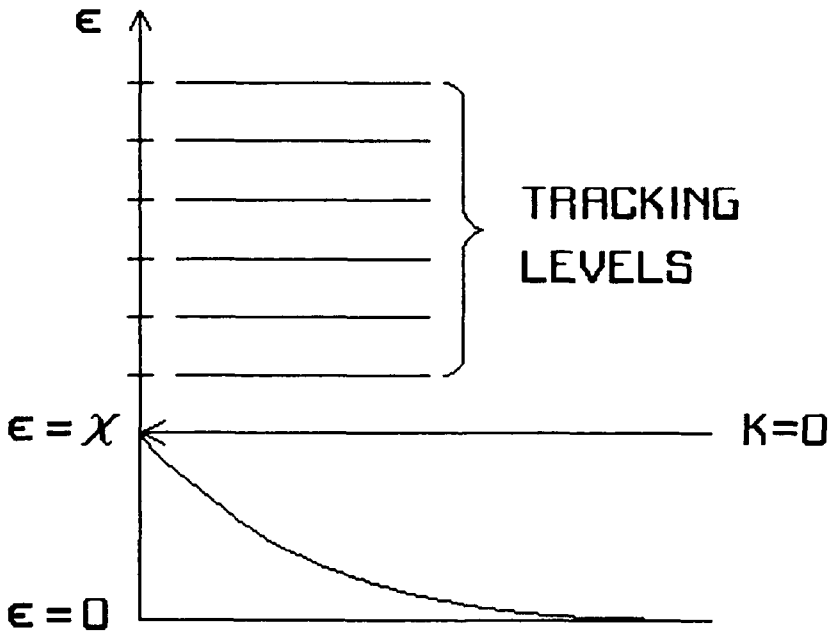

Figure 2. Energy binning for repulsive potentials

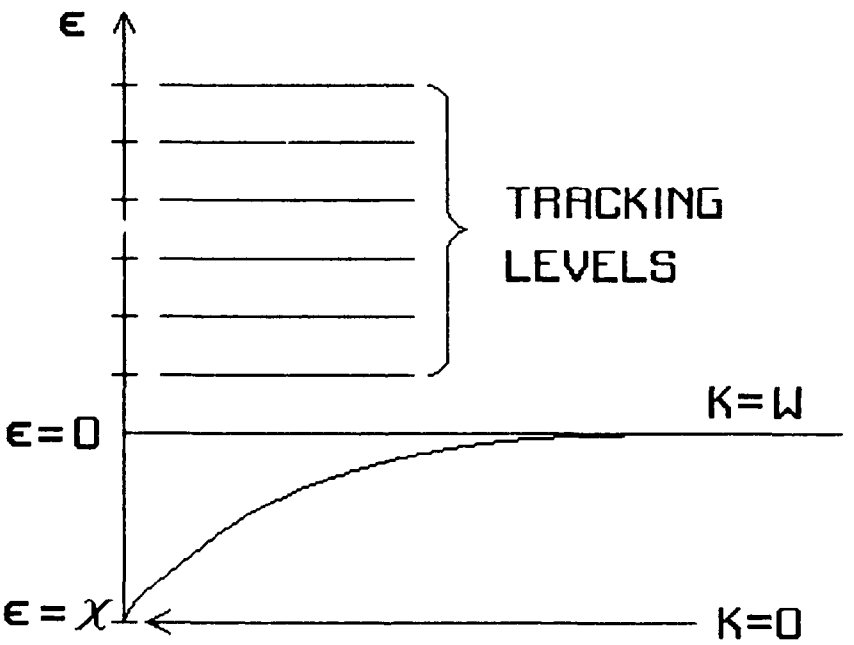

Figure 3. Energy binning for attractive potentials

3. THE TRAPPED ELECTRON MODEL

It is convenient to make a transformation from ϵ to kinetic energy k as the integration variable, then the density integral becomes

$$n = \frac{1}{2}\pi^{-3/2}\iiint \exp(-X)\,k^{1/2}\,dk\,d\Omega$$

where the integration limits on k are

$$\begin{array}{rlll} \textit{repulsion:} & 0 \le k \le \infty & & \\ \textit{attraction:} & 0 \le k \le w & \textit{for trapped particles} & \\ & w \le k \le \infty & \textit{for Vlasov particles} & \end{array}$$

where $w = -\chi > 0$ is the dimensionless well depth. The variable k is also indicated in Figure 2.

For attractive potentials $(\chi < 0)$ we can build a trapped particle model for the kinetic energy range $0 \le k \le w$ by making two assumptions:

1) The source is isotropic $(M = 0)$. Hence, $X = \epsilon = k + \chi$ and the density integral becomes

$$n = \frac{1}{2}\pi^{-3/2}\exp(-\chi)\iiint \exp(-k)\,k^{1/2}\,dk\,d\Omega$$

2) All particles escape. Thus, we can integrate over solid angle so that we have $\iint d\Omega = 4\pi$.

Putting these two assumptions together gives

$$n_t = \exp(-\chi)\cdot\alpha(w)$$

where we define

$$\alpha(w) = 2\pi^{-1/2}\int_0^w \exp(-k)\,k^{1/2}\,dk$$

In the above equations, we have implicitly assumed that the temperature of the trapped and untrapped populations are the same. This is an approximation, since the higher energy particles are preferentially scattered out of the well, leaving a lower temperature for the trapped component.

To illustrate our normalization, consider for a moment the case of repulsive potentials $(\chi > 0)$. The only change would be that the limits on the k integration would be 0 to ∞ and we would have

$$\alpha(\infty) = 2\pi^{-1/2} \cdot \Gamma\left(\frac{3}{2}\right) = 1 \ .$$

so that we would recover the Boltzmann equation for electron density.

We can also, in this manner, make a crude approximation for the Vlasov electrons in the range $w \leq k \leq \infty$. We here keep assumption 1) above, but weaken 2) to: the solid angle for escape is independent of k. This gives

$$n_v = \exp(-\chi) \cdot \beta(w) \cdot g_e$$

$$\beta(w) = 2\pi^{-1/2} \int_w^\infty \exp(-k) k^{1/2} dk$$

The quantity g_e is the solid angle normalized to 4π

$$g_e = \iint d\Omega/(4\pi)$$

which is also equivalent, for an isotropic source, to the neutral particle density. This type of approximation works best, of course, for straight line tracks, i.e. for high velocities and weak electric fields. Since $\alpha(w) + \beta(w) = 1$, we can write n_v in the form

$$n_v = \exp(-\chi) \cdot (1 - \alpha(w)) \cdot g_e$$

This expression is very approximate. However, in our MIP simulations, it makes only a small contribution over most of the chamber (since g_e drops off as $1/r^2$) and we have used it because it avoids the large CPU time required to track the Vlasov electrons.

In the above treatment, the electron density is normalized to 1. at the source, which is the same as for the ion density. This is the correct boundary condition for space conditions, but is not a good approximation for our plasma chamber simulations. There, we have an ion thruster which produces a plasma stream at the front of the chamber, and a hot wire filament located just in front of the ion gun which provides isotropic electrons by emitting an approximately equal current. Thus, we have used a current balance condition to set the normalization of the electron density. We write the total electron density as $n = n_t + n_v$ where

$$n_t = c_t \cdot \exp(-\chi) \cdot \alpha(w)$$

$$n_v = c_v \cdot \exp(-\chi) \cdot (1 - \alpha(w)) \cdot g_e$$

Here, c_t and c_v are separate normalization constants. The value of c_v relative to the ions is determined by approximate flux balance at the source region:

$$Flux_i = N_i \cdot v_s = Flux_e = 1/4\, N_e \cdot \bar{v}_e$$

and therefore

$$c_v = N_e/N_i \cdot 4 v_s/\bar{v}_e = 2\pi^{1/2} M_i (T_i/T_e)^{1/2} (m_e/m_i)^{1/2}$$

where $M_i = v_s/v_i$ is the ion Mach number, T_i, T_e are temperatures, m_i, m_e are masses, and v_e, v_i are thermal velocities (equal to $(2kT/m)^{1/2}$) and $\bar{v}_e = 2\pi^{-1/2} v_e$ denotes average velocity. Assuming the potential is zero at the source, the constant c_t is undetermined by this condition, since $\alpha(0) = 0$. This constant is thus a free parameter in our model. Since the trapped electron source is indirectly that of the neutralizing filament, we expect that c_t would be some fraction of c_v.

4. NUMERICAL RESULTS

In order to show the effects of the model, we have integrated the function $\alpha(w)$ for various well depths. This trapping function $\alpha(w)$ is given in Figure 4. We can see that the function rises rapidly from zero to one in about 6 kT_e. In Figure 5, the trapped electron density n_t calculated assuming unit normalization is shown. This curve shows an even faster rise with respect to w due to the exponential factor $exp(w)$. It is apparent that it only takes a potential well of a few kT_e depth to produce electron densities comparable to that of the ions. This is the mechanism by which positive space charge at the throat of the chamber is effecuvely neutralized. Without this strong negative trapped orbit contribution to the density, one tends to get an unrealistic and unstable build up of positive charge.

To illustrate the numerics, we show below some results for the MIP simulation with -5KV probe. The measured electrostatic potentials are shown in Figure 6. The spherical probe is situated at $Z = 1.0$, $R = 0.$, behind an uncharged front disk centered at $Z = 0$. We see that experimentally, the potential drops off from high negative values near the probe to zero, and then goes positive. We interpret these positive potentials as due to the trapped electrons in balance with the streaming ions. The potential is approximately +4 Volts at the upstream side of the disk. The 4 Volt contour follows the drift direction downstream (toward positive Z) on both sides of the probe. For the MIP experiment $kT_e = 5$ eV, and this contour corresponds to a dimensionless well depth of about $w = -\chi = 4/5$. From Figure 4, we see that this gives a trapping fraction of ~0.35, and from Figure 5, an un-normalized electron density of ~0.75.

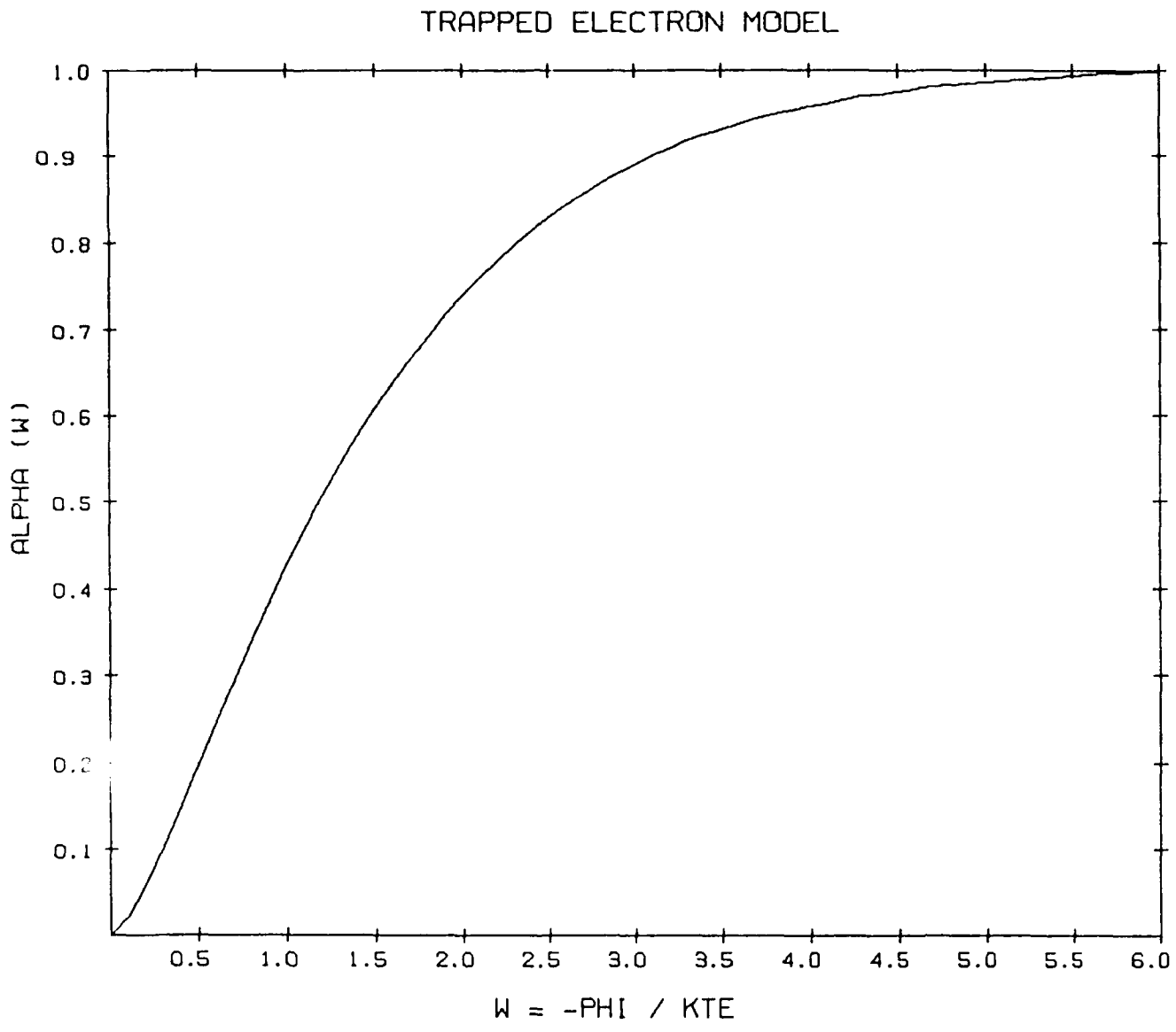

Figure 4. Trapped electron well function alpha(w)

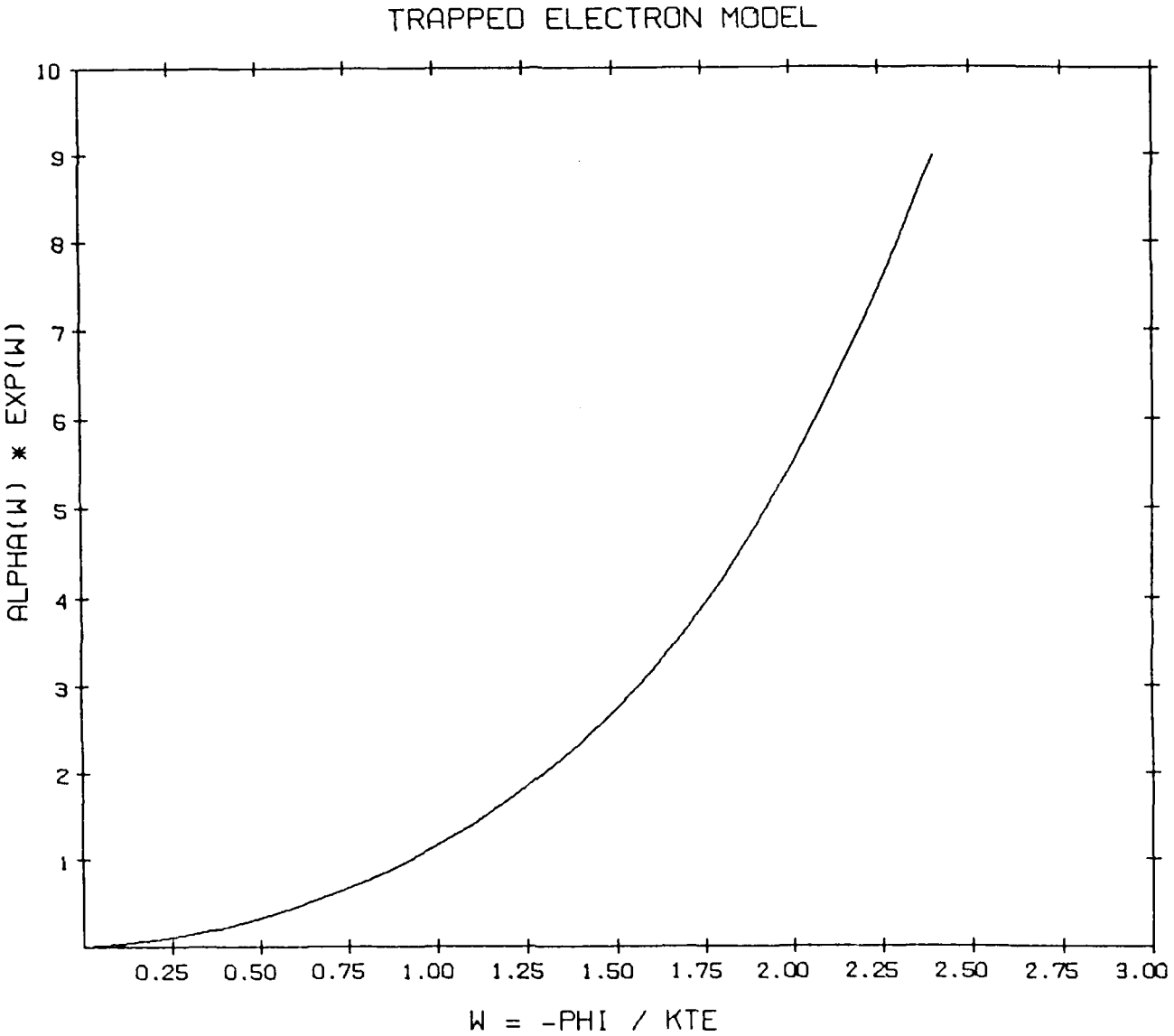

Figure 5. Trapped electron density alpha(w) · exp(w)

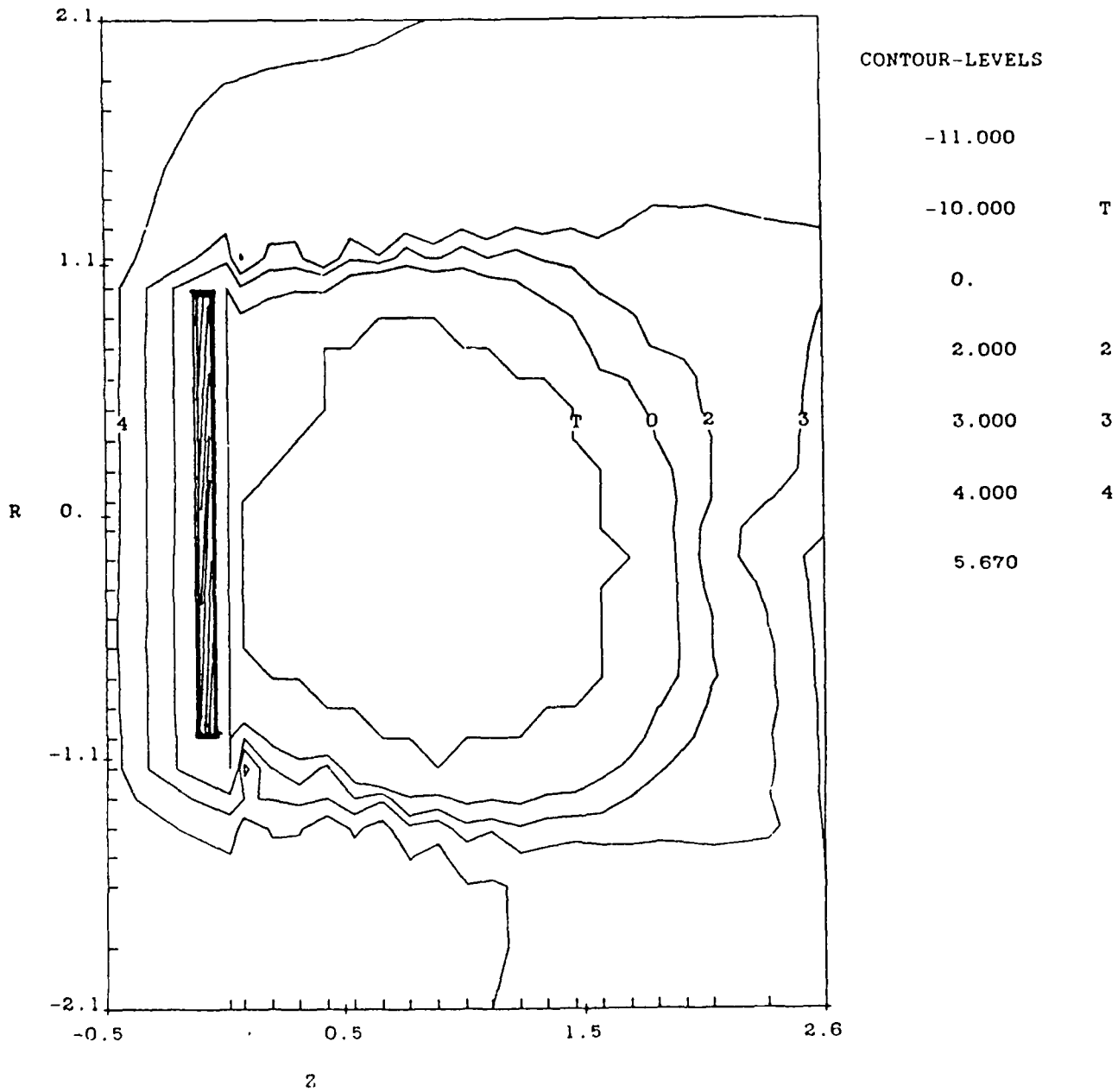

Figure 6. MIP potentials measured with an XY emissive probe

For Argon (40 AMU) flowing at approximately Mach number 3, the current balance condition yields

$$c_v = 2\pi^{1/2} * 3 * 2^{1/2} / (40 * 1832)^{1/2} \sim 0.06$$

The normalized trapped electron contribution, assuming $c_t = c_v$ would be

$$n_t \sim 0.06 * 0.75 \sim 0.05$$

This is of the right order of magnitude, but as expected, is found to be too high to match the ion density at this point. To fine tune the problem, we have taken the value of the free parameter c_t to be less than c_v, the approximate percentage being determined by the best fit to the measured data. Figures 7, 8, 9, and 10 show the Poisson solutions with fixed ion density and a floating trapped electron term, and with normalization set at 20, 30, 40, and 50% of c_v. These Figures indicate the sensitivity of the solutions to the trapped electron normalization constant. As the normalization factor is increased, a shallower potential well is required to bring in the same negative charge, and the positive potentials thereby tend to decrease, as can be seen in Figures 7 to 10. It appears that a value of 30% gives the best match to experimental values around the region of the probe, although a precise comparison cannot be made due to the observed asymmetry in measured potentials. Since MACH is an axisymmetric code, this asymmetry does not appear in the simulations.

5. CONCLUSIONS

In our MACH simulations of the MIP experiment, we have found that the neglect of electron collisional effects leads to unphysical build up of positive charge near the throat of the chamber. We have described a trapped electron model which we have developed to suppress this positive charge. Physically, we assume that chamber electrons can scatter into the potential well created by the ion space charge. The electrons thermalize, with temperature equal to that of the untrapped electrons. The numerical effect of the algorithm is as follows: Whenever the local potential goes positive, that region receives a flood of negative charge due to electrons that fall into the potential well. This quenches any unphysical build up of positive potential. The well depth adjusts so that a self-consistent Poisson-Vlasov solution is obtained. The model contains one free parameter which is the normalization constant for the trapped electron density. The method requires the calculation of numerical quadratures, but no particle tracking. This trapped electron model has been applied to the MACH simulations of the MIP chamber experiment, and enables us to achieve stable solutions with potential distributions that are close to the measured ones.

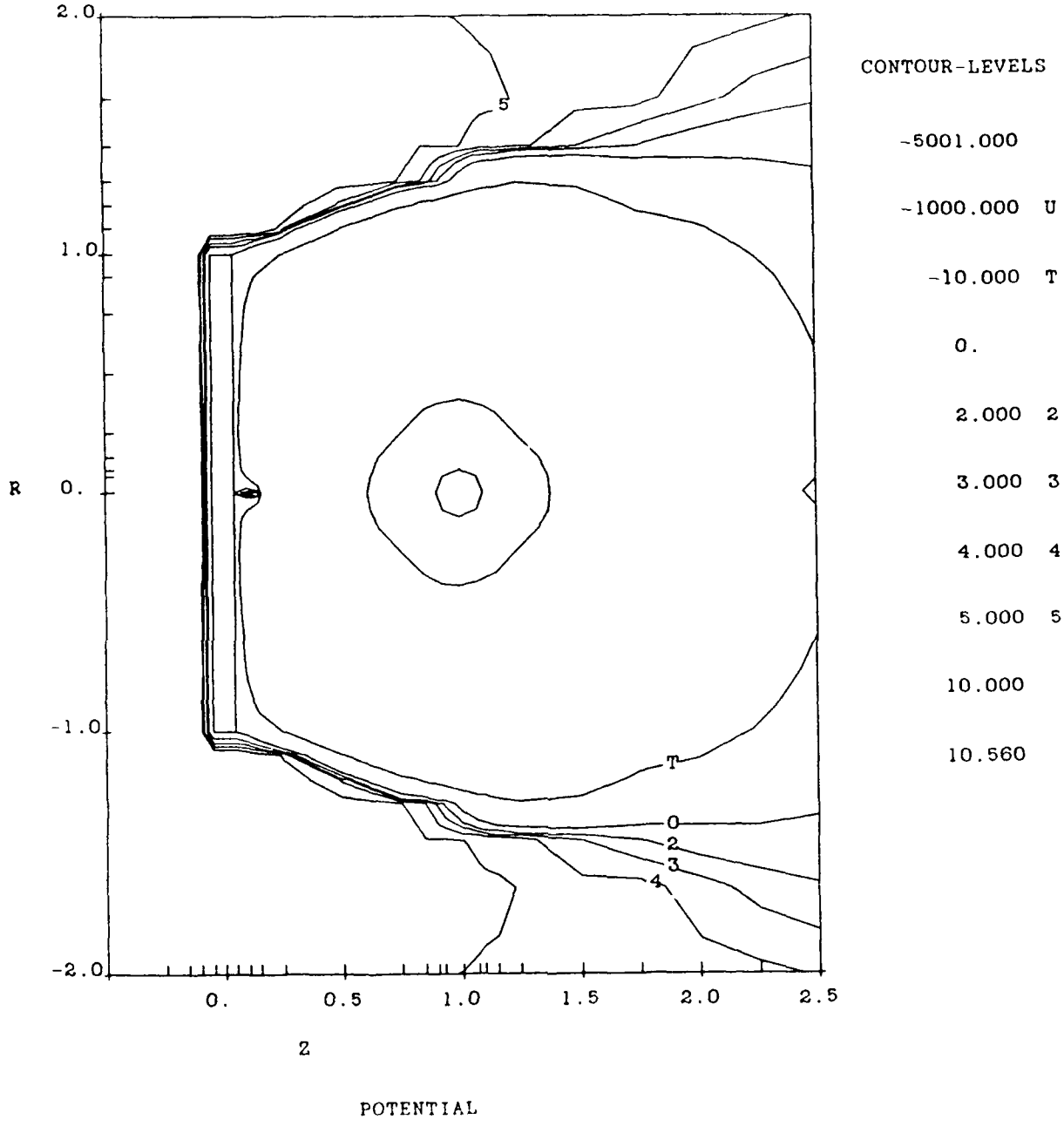

Figure 7. MACH simulation potentials, 20% trapped electrons

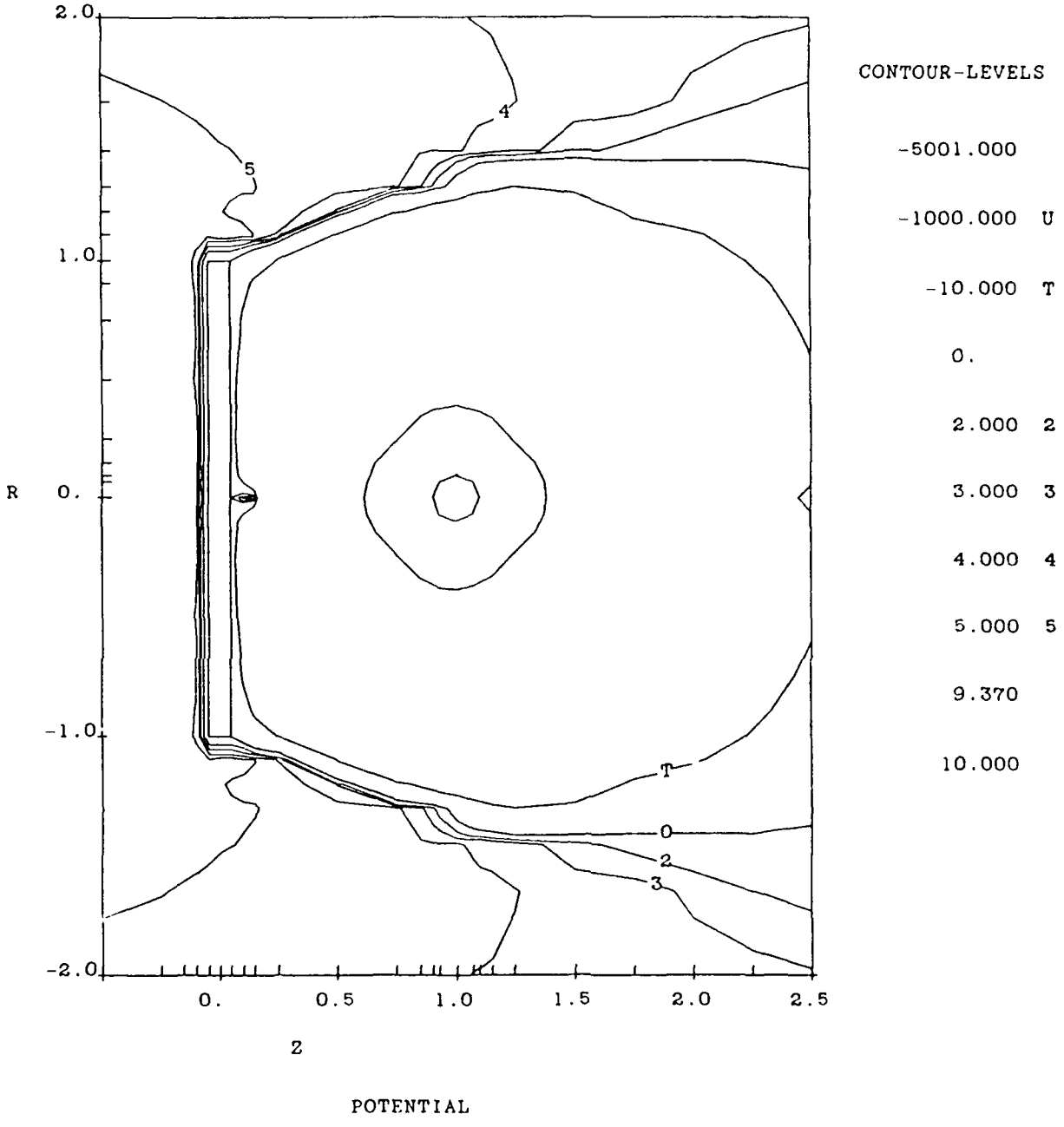

Figure 8. MACH simulation potentials, 30% trapped electrons

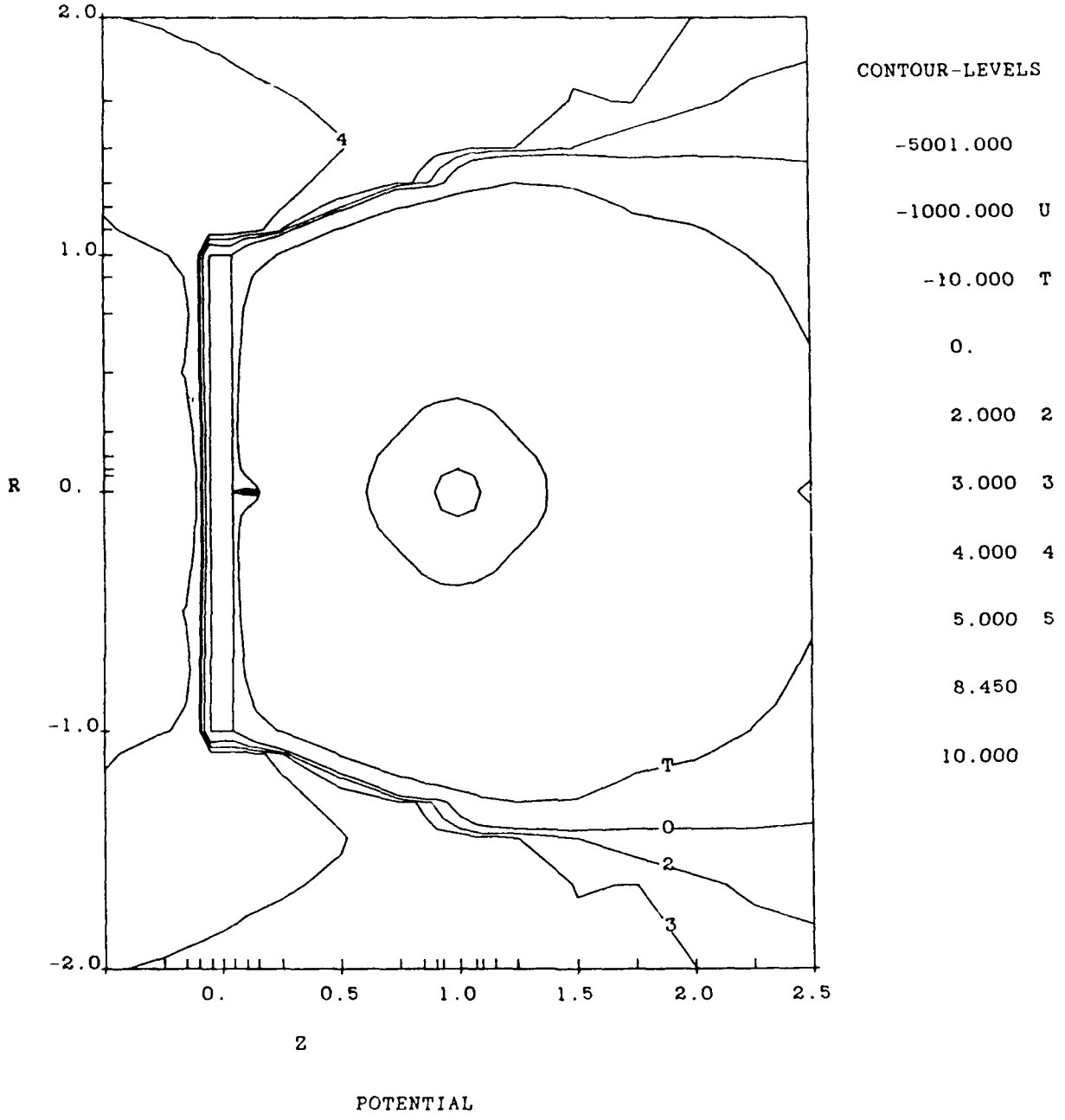

Figure 9. MACH simulation potentials, 40% trapped electrons

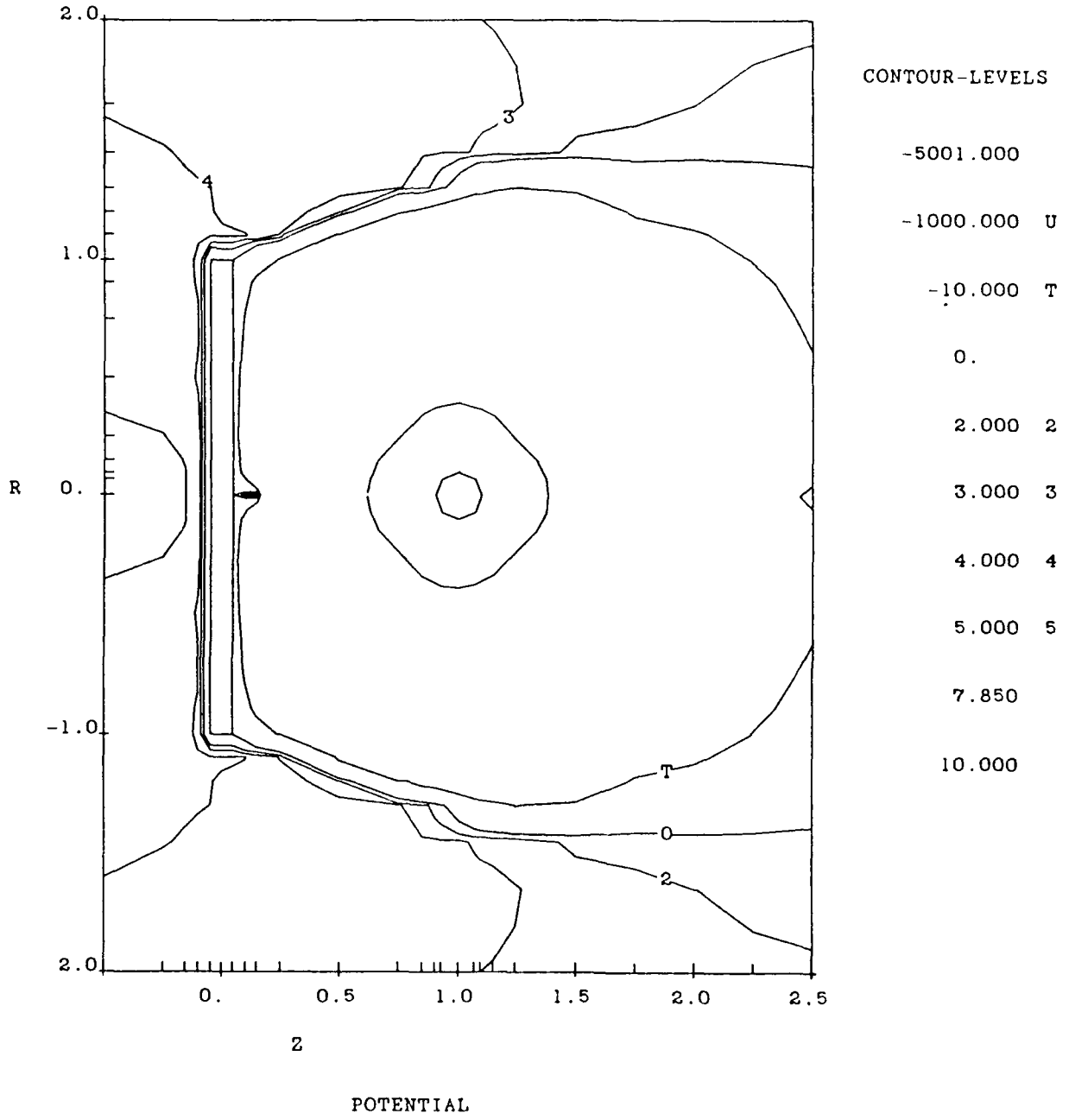

Figure 10. MACH simulation potentials, 50% trapped electrons

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